Effect of disorder on the NMR relaxation rate in two-band superconductors

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We calculate the effect of nonmagnetic impurity scattering on the spin-lattice relaxation rate in two-band superconductors with the s-wave pairing symmetry. It is found that for the interaction parameters appropriate for MgB_2 the Hebel-Slichter peak is suppressed by disorder in the limit of small interband impurity scattering rate. In the limit of strong impurity scattering, when the gap functions in the two bands become nearly equal, the single-band behavior is recovered with a well-defined coherence peak just below the transition temperature.

I. INTRODUCTION

The discovery of superconductivity in MgB_2 [1] has revived the interest in two-band superconductors [2, 3]. Most experiments on this compound [4] are consistent with two distinct superconducting gaps Δ_π and Δ_σ, with $\Delta_\sigma/\Delta_\pi \simeq 2.63$ [5]. The only exception seems to be the nuclear magnetic resonance (NMR) relaxation rate T_1^{-1} [6, 7] in the superconducting state. The NMR relaxation rate measurements on ^{11}B nucleus by Kotegawa *et al.* [6, 7] found a small Hebel-Slichter coherence peak [8] just below the superconducting transition temperature T_c, although there are some questions as to whether the peak is present at all [9, 10]. Moreover, by assuming that the contributions to the relaxation rate from the two bands are simply additive Kotegawa *et al.* found [7] a better fit to their data on ^{11}B nuclei by assuming that only one band participates in the nuclear relaxation process.

In a recent work [11] we have examined the NMR relaxation rate in both conventional and unconventional *clean* two-band superconductors. The essence of our findings is that if the Fermi contact interaction between the nucleus and the conduction electrons dominates the relaxation mechanism, then the measurements of T_1^{-1} probe the properties of the electron subsystem which are local in real space and hence extremely non-local in the momentum space [12]. We showed that for a two-band superconductor this gives rise to inter-band interference terms in T_1^{-1}, in addition to direct contributions from each band.

Here we consider the effect of nonmagnetic impurity scattering on T_1^{-1} for a two-band superconductor. It is well known [13, 14, 15, 16] that the interband scattering by nonmagnetic impurities reduces the transition temperature of an s-wave two-band superconductor. In the case of MgB_2 it has been argued [17] that one requires defects which produce lattice distortions in order to achieve large enough interband scattering which would lead to a significant suppression of T_c. Experimentally, such reduction of T_c was observed on samples of MgB_2 irradiated by fast neutrons [18, 19, 20, 21]. However, there is a finite interband scattering by impurities even in unirradiated and undoped MgB_2 as evidenced by the break-junction tunneling experiments [22] whose interpretation was es-

sentially based on the work of Schopohl and Scharnberg [23] on the tunneling density of states of a disordered two-band superconductor. The interband scattering rate from the low gap band to the high gap band used to fit the tunneling data in [22] was comparable to the transition temperature of 39 K. Thus it seems reasonable to investigate the effect of disorder on T_1^{-1} over a wide range of scattering rates.

The NMR relaxation rate in a superconductor is determined by both normal and anomalous local density of states. In the case of a two-band superconductor these quantities depend on the interband scattering [13, 16, 23] and on temperature [16] in a rather complex way and one cannot a priori guess the effect of disorder on the temperature dependence of T_1^{-1} except in the limits of a small and very large interband impurity scattering rate. In the former case the peaks in the partial densities of states are somewhat reduced and broadened by the interband scattering compared to the clean system and one would expect the Hebel-Slichter coherence peak in T_1^{-1} below T_c to be reduced and broadened by disorder. In the limit of a very large interband scattering such that the gap functions in the two bands become nearly equal (the Anderson limit [24]), the difference between the local densities of states in the two bands has no consequences and one expects to find the temperature dependence of T_1^{-1} characteristic of a single-band superconductor, with the size of the Hebel-Slichter peak determined by the strength of the electron-phonon coupling in the system [25, 26]. In the case of MgB_2, which is a medium coupling superconductor [5], the Hebel-Slichter peak is expected to be quite large in the Anderson limit. Indeed we find that our detailed numerical calculations of T_1^{-1} over a wide range of the interband impurity scattering rates confirm such a trend.

The rest of the article is organized as follows. In Sec. II, we summarize the strong coupling theory of the NMR relaxation rate in a disordered s-wave two-band superconductor assuming that the Fermi contact interaction between the nuclear spin and the conduction electrons provides the dominant relaxation mechanism. In Sec. III we give the results of our numerical calculations using the interaction parameters for MgB_2 [5, 14, 27] and in Sec. IV we give conclusions.

II. THEORY

The relaxation rate of a nuclear spin due to the hyperfine contact interaction with the band electrons is given by [11]

$$R \equiv \frac{1}{T_1 T} = -\frac{J^2}{2\pi} \lim_{\omega_0 \to 0} \frac{\text{Im} \, K^R_{+-}(\omega_0)}{\omega_0}, \qquad (1)$$

where J is the hyperfine coupling constant, ω_0 is the NMR frequency, and $K^R_{+-}(\omega_0)$ is the analytic continuation of the Fourier transform $K(\nu_m)$ of the imaginary time correlator

$$K(\tau) = -\langle\langle T_\tau (S_+(\mathbf{0}, -i\tau) S_-(\mathbf{0}, 0))\rangle\rangle_i \qquad (2)$$

averaged over the impurity configurations. Here $S_\pm(\mathbf{r}, -i\tau) = e^{H_e \tau} S_\pm(\mathbf{r}) e^{-H_e \tau}$, H_e is the electron Hamiltonian, and

$$S_+(\mathbf{r}) = \psi^\dagger_\uparrow(\mathbf{r})\psi_\downarrow(\mathbf{r}), \quad S_-(\mathbf{r}) = \psi^\dagger_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r}) \qquad (3)$$

with $\psi^\dagger_\sigma(\mathbf{r})$ and $\psi^\dagger_\sigma(\mathbf{r})$ being the electron field operators ($\hbar = k_B = 1$ in our units, and we consider a system of unit volume). H_e contains both electron-phonon and screened Coulomb interactions as well as the scattering off randomly located nonmagnetic impurities.

We assume that there are two spin-degenerate electron bands in the crystal (the generalization to an arbitrary number of bands is straightforward), and neglect the spin-orbit coupling. Then the spin operators (3) can be written in the band representation, using

$$\psi_\alpha(\mathbf{r}) = \sum_{i,\mathbf{k}} e^{i\mathbf{k}\mathbf{r}} u_{i,\mathbf{k}}(\mathbf{r}) c_{i,\mathbf{k}\alpha} , \qquad (4)$$

where $u_{i,\mathbf{k}}(\mathbf{r})$ are the Bloch functions, which are periodic in the unit cell. Inserting these into Eqs. (3), one obtains

$$\begin{aligned} K(\nu_m) &= \frac{1}{2} T \sum_n \sum_{\mathbf{k}_1 \mathbf{k}_2} \sum_{i,j} |u_{i,\mathbf{k}_1}(\mathbf{0})|^2 |u_{j,\mathbf{k}_2}(\mathbf{0})|^2 \\ &\times \text{Tr} \, [\hat{G}_i(\mathbf{k}_1, \omega_n) i\tau_2 \hat{G}_j(\mathbf{k}_2, -(\omega_n + \nu_m)) \\ &\times \hat{\Gamma}_{ij}(\mathbf{k}_1, \mathbf{k}_2; \omega_n, \nu_m)] , \end{aligned} \qquad (5)$$

where $\hat{G}_i(\mathbf{k}, \omega_n)$ are the impurity-averaged Green's functions given by

$$\hat{G}_i(\mathbf{k}, \omega_n) = -\frac{i\omega_n Z_i(\omega_n)\tau_0 + \xi_{i,\mathbf{k}}\tau_3 + \phi_i(\omega_n)\tau_1}{\omega_n^2 Z_i^2(\omega_n) + \xi_{i,\mathbf{k}}^2 + \phi_i^2(\omega_n)} . \qquad (6)$$

Here $Z_i(\omega_n)$ and $\phi_i(\omega_n)$ are the renormalization function and the pairing self-energy, respectively, for the ith band.

In Ref. [11] we argued that the contribution to the vertex functions $\hat{\Gamma}_{ij}(\mathbf{k}_1, \mathbf{k}_2; \omega_n, \nu_m)$ from the electron-phonon interaction can be ignored while the effect of the Coulomb interaction drops out from the ratio R_s/R_n. In calculating the contibution to $\hat{\Gamma}_{ij}$ from the impurity scattering in the conserving approximation [28] one considers only the ladder impurity diagrams since the self-energies are calculated in the self-consistent second Born approximation. We have shown recently [29] that in the case of a single three-dimensional band the contribution to the vertex function $\hat{\Gamma}$ from the ladder impurity diagrams is of the order γ/ϵ_F, where γ is the impurity scattering rate and ϵ_F is the Fermi energy, and that the impurity vertex corrections can therefore be neglected. The same applies to the contribution to $\hat{\Gamma}_{ij}$ from the ladder impurity diagrams since the structure of the impurity ladder diagrams for the $\hat{\Gamma}_{ij}$s is completely analogous to the single-band case. Hence, we replace $\hat{\Gamma}_{ij}$ in Eq. (5) with matrix $i\tau_2$ in computing the ratio of the spin-lattice relaxation rates in the superconducting and normal states.

Next, by introducing the spectral representation for $\hat{G}_i(\mathbf{k}, \omega_n)$ one can calculate the Matsubara sums in Eq. (5) and then analytically continue the result to just above the real frequency axis $i\nu_m \to \omega_0 + i0^+$ [11]. In the limit $\omega_0 \to 0$ we obtain

$$\frac{R_s}{R_n} = 2 \int_0^{+\infty} d\omega \left(-\frac{\partial f}{\partial \omega}\right) \frac{N^2(\omega) + M^2(\omega)}{N_n^2} , \qquad (7)$$

where the densities of states (both normal and anomalous) are defined by

$$N(\omega) = \sum_i N_{n,i} \text{Re} \frac{\omega}{\sqrt{\omega^2 - \Delta_i^2(\omega)}} , \qquad (8)$$

$$M(\omega) = \sum_i N_{n,i} \text{Re} \frac{\Delta_i(\omega)}{\sqrt{\omega^2 - \Delta_i^2(\omega)}} . \qquad (9)$$

Here

$$N_{n,i} = N_{F,i} \left\langle |u_{i,\mathbf{k}}(\mathbf{0})|^2 \right\rangle_i \qquad (10)$$

are the local densities of states at the nuclear site in the normal state, with $N_{F,i}$ the Fermi level density of states in ith band, $N_n = N_{n,1} + N_{n,2}$, and $\Delta_i(\omega) = \phi_i(\omega)/Z_i(\omega)$ is the gap function in ith band.

The gap functions are obtained by solving the finite temperature Eliashberg equations on the real axis [30], which include the electron-phonon interaction, screened Coulomb repulsion and both the interband and intraband impurity scattering described by the self-consistent

second Born approximation:

$$\phi_i(\omega) \;=\; \phi_i^0(\omega) + i\sum_j \frac{\gamma_{ij}}{2}\frac{\Delta_j(\omega)}{\sqrt{\omega^2 - \Delta_j^2(\omega)}}\;, \qquad (11)$$

$$\phi_i^0(\omega) \;=\; \sum_j \int_0^{\omega_c} d\omega'\,\mathrm{Re}\,\frac{\Delta_j(\omega')}{\sqrt{\omega'^2 - \Delta_j^2(\omega')}}$$
$$\times\,[f(-\omega')K_{+,ij}(\omega,\omega') - f(\omega')$$
$$\times\,K_{+,ij}(\omega,-\omega') - \mu_{ij}^*(\omega_c)\tanh\frac{\omega'}{2T}$$
$$+\,K_{+,ij}^{TP}(\omega,\omega') - K_{+,ij}^{TP}(\omega,-\omega')]\;, \qquad (12)$$

$$Z_i(\omega) \;=\; Z_i^0(\omega) + i\sum_j \frac{\gamma_{ij}}{2}\frac{1}{\sqrt{\omega^2 - \Delta_j^2(\omega)}}\;, \qquad (13)$$

$$Z_i^0(\omega) \;=\; 1 - \frac{1}{\omega}\sum_j \int_0^{+\infty} d\omega'\,\mathrm{Re}\,\frac{\omega'}{\sqrt{\omega'^2 - \Delta_j^2(\omega')}}$$
$$\times\,[f(-\omega')K_{-,ij}(\omega,\omega') - f(\omega')K_{-,ij}(\omega,-\omega')$$
$$+\,K_{-,ij}^{TP}(\omega,\omega') + K_{-,ij}^{TP}(\omega,-\omega')]\;, \qquad (14)$$

where

$$K_{\pm,ij}(\omega,\omega') = \int_0^{+\infty} d\Omega\,\alpha^2 F_{ij}(\Omega)$$
$$\times\left[\frac{1}{\omega'+\omega+\Omega+i0^+} \pm \frac{1}{\omega'-\omega+\Omega-i0^+}\right], \qquad (15)$$

$$K_{\pm,ij}^{TP}(\omega,\omega') = \int_0^{+\infty} d\Omega\,\frac{\alpha^2 F_{ij}(\Omega)}{e^{\Omega/T}-1}$$
$$\times\left[\frac{1}{\omega'+\omega+\Omega+i0^+} \pm \frac{1}{\omega'-\omega+\Omega-i0^+}\right]. \qquad (16)$$

Here $\alpha^2 F_{ij}(\Omega)$ and $\mu_{ij}^*(\omega_c)$ are intraband and interband electron-phonon coupling functions and Coulomb repulsion parameters for the cutoff ω_c, respectively. The impurity scattering rates are defined by $\gamma_{ij}/2 = n_{imp}\pi N_{F,j}(0)|V_{ij}|^2$ where n_{imp} is the concentration of impurities and V_{ij} is the Fermi surface averaged matrix element of the change in the lattice potential caused by an impurity between the states in the bands i and j.

It is easy to see that the intraband scattering rates γ_{ii} drop out from the equations for the gap functions $\Delta_i(\omega) = \phi_i(\omega)/Z_i(\omega)$ which are obtained from Eqs. (11-14), and only the interband impurity scattering affects the gap functions and hence R_s/R_n, Eqs. (7-9). We should point out that the Eqs. (11-14) are the same as the strong coupling equations for the McMillan tunneling model of the superconducting proximity effect [31] and were first solved numerically at zero temperature by Zarate and Carbotte [32] over twenty years ago.
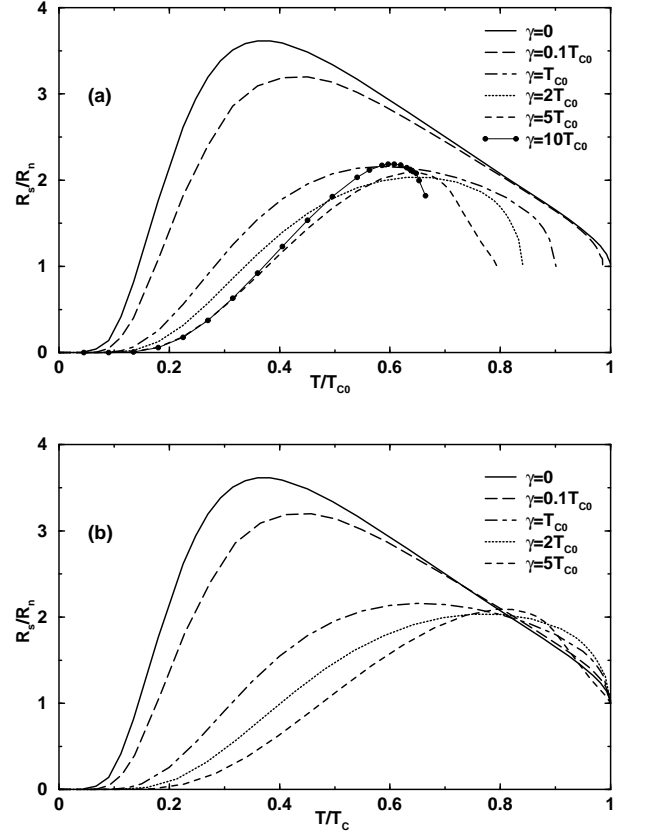

FIG. 1: The ratio R_s/R_n in the case when the relaxation is dominated by the lower-gap band ($N_{n,\sigma}=0$) for several values of the interband scattering rate $\gamma_{\pi\sigma} \equiv \gamma$ in the units of transition temperature of the clean system T_{c0}. In (a) R_s/R_n is plotted as a function of temperature in units of T_{c0}. Note that for $\gamma/T_{c0}=10$ the results do not extend all the way to the transition temperature T_c because of the poor convergence of the real-axis Eliashberg equations near T_c for such a high value of γ. In (b) R_s/R_n is plotted as a function of T/T_c, where T_c is the transition temperature of disordered system, in order to illustrate the change in the relative width and position of the coherence peaks with increasing γ.

III. RESULTS

In order to examine the effect of the interband impurity scattering on the NMR relaxation rate of a singlet two-band superconductor we have calculated R_s/R_n for the interaction parameters of MgB$_2$. The four electron-phonon coupling functions $\alpha^2 F_{ij}(\Omega)$, $i,j = \sigma,\pi$, were calculated by Golubov *et al.* [5] and the Coulomb repulsion parameters $\mu_{ij}^*(\omega_c)$ were determined in [14, 27] based on the screened Coulomb repulsion parameters of MgB$_2$ calculated by Choi *et al.* [33]. Since $\gamma_{\sigma\pi}/\gamma_{\pi\sigma} = N_{F,\pi}/N_{F,\sigma}$ there is only one independent interband scattering rate parameter and we choose $\gamma_{\pi\sigma} \equiv \gamma$. Our representative results are shown in Figs. 1 and 2. Figure 1 is our theoretical prediction for the relaxation rates on ^{25}Mg nuclei in MgB$_2$, for which the dominant relaxation mechanism is
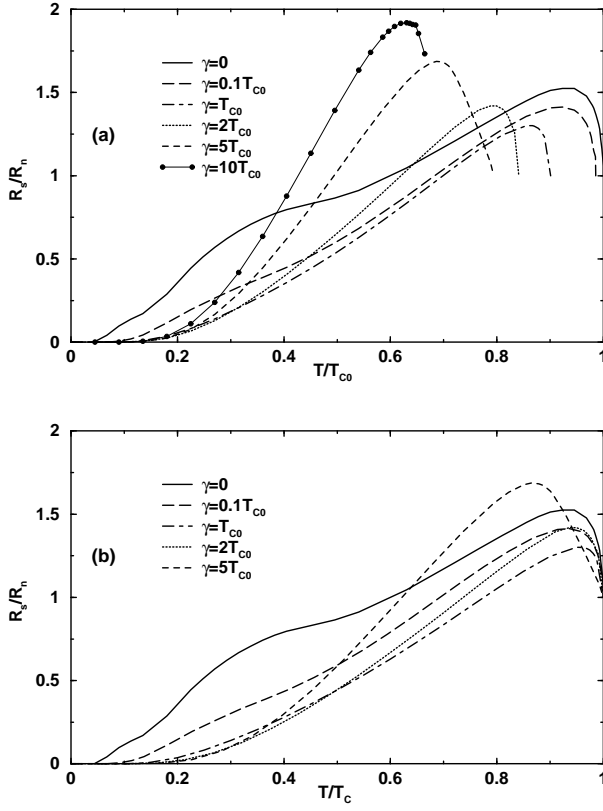
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FIG. 2: The ratio R_s/R_n for $N_{n,\pi}/N_{n,\sigma}=0.45$ for several values of the interband scattering rate $\gamma_{\pi\sigma} \equiv \gamma$ in the units of the transition temperature of the clean system T_{c0}. In (a) R_s/R_n is plotted as a function of temperature in units of T_{c0}. In (b) R_s/R_n is plotted as a function of T/T_c, where T_c is the transition temperature of disordered system.

FIG. 3: The densities of states, $\mathrm{Re}\left[\omega/\sqrt{\omega^2 - \Delta_{\sigma,\pi}(\omega)}\right]$, in the σ and π bands at (a) $T = 0$ and (b) $T = 0.95T_c$, for the impurity interband scattering rates $\gamma = 0.1T_{c0}$ and $\gamma = T_{c0}$.

the Fermi contact interaction [34, 35] and the electronic structure calculations [36] give $N_{n,\sigma} \approx 0$ for the Mg-site. To the best of our knowledge there are no measurements of $1/T_1$ in the superconducting state on ^{25}Mg in MgB$_2$, presumably because of its small magnetic moment and a low natural abundance, but the experiments performed in [37, 38] indicate that it is possible to measure ^{25}R below the superconducting transition temperature. Such measurements would be highly desirable since our theory is quantitatively correct for ^{25}Mg nucleus. The broad peaks in Fig. 1 between $0.3T_c$ and $0.6T_c$ for $0\leq \gamma \leq 2T_c$ are analogous to the broad peaks found in the microwave conductivity of MgB$_2$ [39] in the same temperature range. In [39] the best fits to the data were obtained by assuming that the π-band gives the dominant contribution to the microwave conductivity and our results in Fig. 1 also give only the π-band contribution to R_s/R_n ($N_{n,\sigma} = 0$). Since both NMR relaxation rate and the microwave conductivity have the same coherence factors in the single band case [40] the similarity between our prediction for ^{25}R and the results obtained in [39] is not accidental.

In Fig. 2 we present our results for $N_{n,\pi}/N_{n,\sigma} = 0.45$, which would correspond to ^{11}B nucleus [36] in MgB$_2$ if
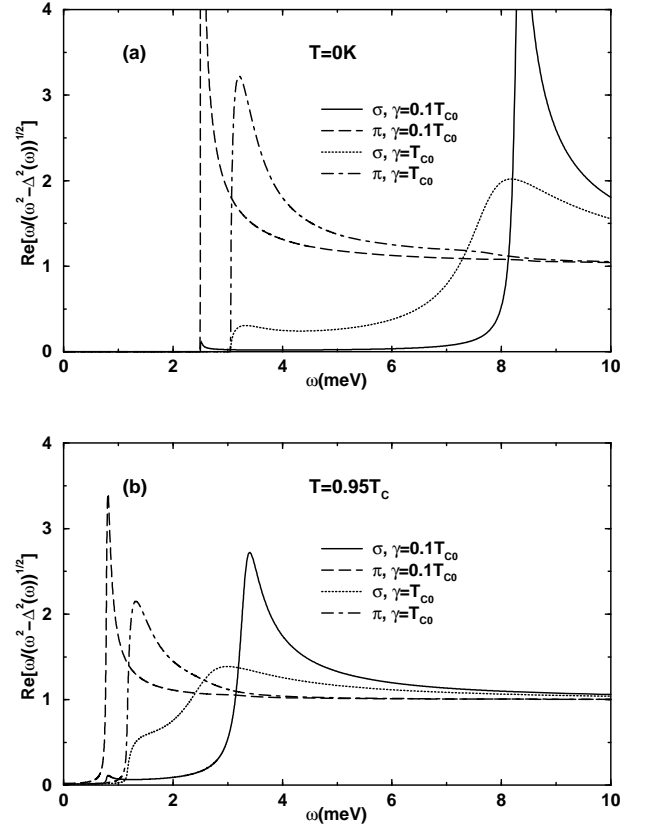
the dominant relaxation mechanism were the Fermi contact interaction. However, the local-density approximation (LDA) calculations [34, 35] have found that at the ^{11}B nucleus the most significant contribution to the relaxation comes from the interaction with the electronic orbital part of the hyperfine field. Hence, our results in Fig. 2 should not be compared directly with the experimental results for ^{11}R. While the predictions in [34, 35] were confirmed by experiments [37, 38, 41] in the *normal* state, until recently [42] nothing was known theoretically about the temperature dependence of $1/T_1$ in a superconductor in which the orbital part of the hyperfine field dominates the NMR relaxation. Our preliminary results [42] for a single band superconductor indicate that in such a case the temperature dependence of R_s/R_n is given by the standard expressions obtained for the Fermi contact interaction [30, 40] provided that γ is much greater than T_c. In our treatment [42] of the orbital contribution to R_s/R_n the extended nature of the single electron states participating in the formation of Cooper pairs played the key role, and it is not clear how the treatment of [34, 35] in which a few localized orbitals are responsible for the orbital part of the hyperfine field could be extended to the superconducting state.

It is apparent from Figs. 1 and 2 that as the inter-

band impurity scattering rate increases initially from 0 to about $2T_{c0}$ the coherence peak in the NMR relaxation rate is reduced and moved closer to the T_c. In the case of ^{25}R the peak is also broadened (see Fig. 1b) while the shoulder in R_s/R_n for $N_{n,\pi}/N_{n,\sigma} = 0.45$ in Fig. 2 for γ=0 resulting from the π-band contribution is rapidly reduced, Fig. 1. As we have anticipated in Sec. I these changes in R_s/R_n at low values of γ are a direct consequence of the changes in both normal and anomalous densities of states in the superconducting state with increasing impurity scattering, Eqs. (7-9). In Fig. 3 we show the partial densities of states in the two bands at $T = 0$ and at T just below the T_c, for two lowest values of the interband impurity scattering parameter γ from Figs. 1 and 2. Clearly, in the low γ regime increasing interband impurity scattering leads to a reduction and smearing of the partial densities of states both at low and high temperatures. As a result the the Hebel-Slichter coherence peaks are reduced in size and in the case of a single-band contribution, Fig. 1, the peak is also broadened.
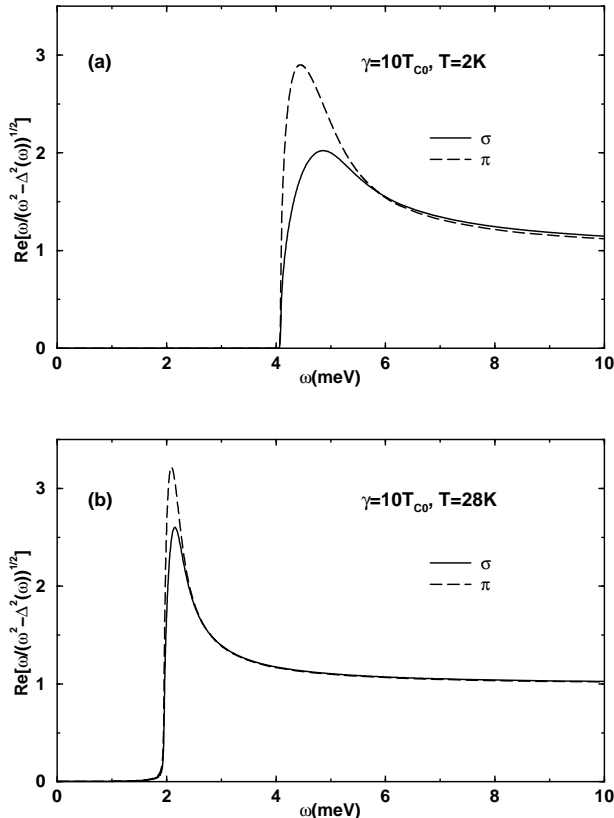

FIG. 4: The densities of states, $\mathrm{Re}\left[\omega/\sqrt{\omega^2 - \Delta_{\sigma,\pi}^2(\omega)}\right]$, in the σ and π bands at (a) $T = 2$ K and (b) $T = 28$ K for the highest impurity interband scattering rates $\gamma = 10T_{c0}$ considered in this work.

At high vales of γ (the Anderson limit) one expects that the gap functions in the two bands will become nearly equal, resulting in nearly equal normal and anomalous densities of states in both bands. As a result one expects the system to display $1/T_1$ characteristic of a single-band superconductor with pronounced Hebel-Slichter peak, barring extremely strong electron-phonon coupling [25, 26]. Indeed, as illustrated in Fig. 4 for $\gamma = 10T_{c0}$, the densities of states in the two bands are very similar, in particular at high temperature where the damping term in Eq. (11) associated with the interband impurity scattering is reduced by the smaller gaps at high temperatures. The corresponding R_s/R_n shown in Figs. 1(a) and 2(a) have well pronounced coherence peaks similar in shape to what one would expect for a single-band s-wave superconductor.

IV. CONCLUSIONS

We calculated the NMR relaxation rate $1/T_1$ in an s-wave two-band superconductor with impurities, assuming that the relaxation of nuclear spins is controlled by the Fermi contact interaction with the band electrons. Using the interaction parameters of MgB_2 [5, 33] we found that for low interband impurity scattering rates disorder suppresses Hebel-Slichter coherence peak as a result of the smearing of the densities of states in the two bands with two different gaps. For high scattering rates, as the gap functions in the two bands become nearly equal, the system behaves as a single-band superconductor with a well-developed coherence peak below T_c, as appropriate for a medium electron-phonon coupling parameter $\lambda \approx 1$ and a small ratio T_c/Ω_{max}, where Ω_{max} is the maximum phonon frequency. However, one should keep in mind that in the limit of strong disorder, such as found in the samples of MgB_2 irradiated with high neutron fluences [18, 19, 20, 21], our treatment of disorder is not sufficient to quantitatively describe all experimental results. Indeed recently observed [19, 20, 21] reduction of the smaller π-band gap with increasing disorder in neutron irradiated samples of MgB_2 can never be reproduced within the self-consistent second Born approximation treatment of impurity scattering used here and elsewhere in the literature on two-band superconductivity. For a highly disordered system one would likely have to consider changes in the electron-phonon interaction and the normal state densities of states to account for the reduction of the gap in three-dimensional π-band.

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